

D-(-)-Mandelic acid
611-71-2 | DTXSID4046523

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 9.93e-06 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.85e-01

Confidence level: 4.22e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>N,N-Dimethylformamide</div> <div>Measured: 8.20e-05</div> <div>Predicted: 5.14</div>	<div>Image not found</div> <div>4-Isopropylphenol</div> <div>Measured: 1.92e-07</div> <div>Predicted: 3.08e-02</div>	<div>Image not found</div> <div>1,2-Benzenedicarbonyl dichloride</div> <div>Measured: 6.36e-07</div> <div>Predicted: 2.89e-03</div>
<div>Image not found</div> <div>Chloridazon</div> <div>Measured: 1.20e-05</div> <div>Predicted: 1.36e-07</div>	<div>Image not found</div> <div>2-Methylbenzothiazole</div> <div>Measured: 3.66e-03</div> <div>Predicted: 2.57e-02</div>	